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Entanglement and quantum phase transition in quantum mixed spin chains

Shang-Bin Li,* Zhao-Xing Xu, Jian-Hui Dai, and Jing-Bo Xu†
Chinese Center of Advanced Science and Technology (World Laboratory), P.O.Box 8730, Beijing, People's Republic of China; and Zhejiang Institute of Modern Physics and Department of Physics, Zhejiang University, Hangzhou 310027, People's Republic of China

The ground entanglement and thermal entanglement in quantum mixed spin chains consisting of two integer spins 1 and two half integer spins $\frac{1}{2}$ arrayed as $\frac{1}{2}-\frac{1}{2}-1-1$ in a unit cell with antiferromagnetic nearest-neighbor couplings $J_1(J_2)$ between the spins of equal (different) magnitudes, are investigated by adopting the log-negativity. The ground entanglement transition found here is closely related with the valence bond state transition, and the thermal entanglement near the critical point is calculated and shown that two distinct behaviors exist in the nearest neighbor same kind of spins and different kind of spins, respectively. The potential application of our results on the quantum information processing is also discussed.

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I. INTRODUCTION

Entanglement, one of the most striking features of quantum mechanics [1], has been recognized as an important resource for quantum information processing [2, 3]. Recently, the entanglement in the systems of condensed matter physics such as the Heisenberg models has cause much attention [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26]. Natural entanglement in the thermal equilibrium of the spin chains coupled by the exchange interaction has been found and it is shown that the temperature or the external magnetic field can enhance the pairwise entanglement of spins [5]. The relations between the ground state entanglement and quantum phase transition have also be revealed for the classes of spin-1/2 chains [8, 10, 11]. All results concerning the entanglement in the Heisenberg spin chains showed that the entanglement can make a bridge across the condensed matter physics and quantum information theory.

One of the most famous results in quantum spin chains is the Haldane conjecture which implies that the half-odd-integer antiferromagnetic Heisenberg chains should have gapless spectrum with algebraic decay of correlations at zero temperature and integer spin ones should be gapped with exponential decay of correlations. Recently, some authors have addressed whether the entanglement length is finite or infinite in the Heisenberg spin-1 chain which is a gapped quantum Hamiltonian and proven the existence of an infinite entanglement length as opposed to their finite correlation length [23]. Besides the spin-1 chains, recent experimental achievements [28, 29, 30] have stimulated the interest to study both analytically and numerically the mixed quantum spin chains, such as the alternating quantum spin chain with $S^1 = 1/2$ and $S^2 = 1$ with antiferromagnetic nearest-neighbor exchange interaction or more complicated hypothetical 1D periodic structures of different spins with ferrimagnetic properties [31]. The topology of spin arrangements in the ferrimagnetic chain plays an essential role on the variation of energy gap associated with Haldane conjecture and on the magnetism of ground states. The ground state of ferrimagnetic chain with two kinds of different spins is either a spin singlet or ferrimagnetic due to the setup of the bipartite lattices following Marshall theorem [32]. By applying the Lieb-Schultz-Mattis theorem [33], one can find whether the ferrimagnetic chains have a gapless excitation though the theorem failed to predict the existence of a gapped excitation. In this Letter, we consider the ground state entanglement and thermal state entanglement in an interesting model which is called as quantum mixed spin 1/2-1/2-1-1 chain by making use of the quantum Monte Carlo method with a improved loop cluster algorithm [34]. Over the past years, the quantum Monte Carlo method with a improved loop cluster algorithm has proven it to be a efficient numerical tool to deal with the complicated coupled spin chains [34, 35]. So it is very credible to numerically investigate the nonclassical properties such as the entanglement of the mixed spin chain by adopting this method.

For first time, we investigate the ground state entanglement of the mixed spin chain up to 128 sites by exploring the log-negativity as an entanglement measure. Two distinct behaviors of pairwise entanglement are found. We provide a evidence that the ground state entanglement between two 1/2 spins or between 1/2 spin and 1 spin are closely related to the so-called VBS phase transition. At the point of VBS phase transition, the ground state between two 1/2 spins can be transferred to two different kinds of spins i.e. the spin 1/2 and spin 1 or vice versa. Furthermore, the thermal state pairwise entan-

*Electronic address: sbli@zju.edu.cn
†Electronic address: phyxujb@mail.hz.zj.cn

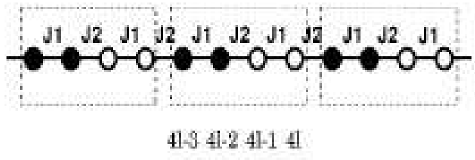

FIG. 1: Graphical representation of the Hamiltonian in Eq.(1), the black and white circles represent spins $\frac{1}{2}$ and 1, respectively.

glement is also studied and whether the thermal entanglement can be improved by increasing the temperature or not is also addressed, which strongly depends on the parameter $\alpha = J_2/J_1$.

This paper is organized as follows: In Sec.II, we briefly outline the basic content of the quantum mixed spin chain and investigate the ground state entanglement between two nearest-neighbor spins $\frac{1}{2}$ or between two nearest-neighbor spins $\frac{1}{2}$ and 1. In Sec.III, we investigate the thermal state entanglement between two nearest-neighbor spins $\frac{1}{2}$ or between two nearest-neighbor spins $\frac{1}{2}$ and 1. It is shown that the entanglement can be enhanced by improve the temperature. In Sec.IV, there are some conclusive remarks.

II. The ground state entanglement and the VBS phase transition of quantum mixed spin chain

Now we consider the quantum antiferromagnetic mixed spin $S^1 - S^1 - S^2 - S^2$ chain displayed by Fig.1, whose Hamiltonian can be given by [35]

$$\begin{aligned} H &= \sum_{n=1}^{N/4}(J_1 S^1_{4n-3}\cdot S^1_{4n-2} + J_2 S^1_{4n-2}\cdot S^2_{4n-1} \\ &\quad + J_1 S^2_{4n-1}\cdot S^2_{4n} + J_2 S^2_{4n}\cdot S^1_{4n+1}). \qquad (1) \end{aligned}$$

Here, the periodic boundary condition is adopted. In the case with $S^1 = \frac{1}{2}$ and $S^2 = 1$, the model has been studied by quantum Monte Carlo (QMC) simulation [36] and the nonlinear σ model (NLSM) [37, 38]. The ground state of this model is nonmagnetic with gapped excitations. The gap varies as a function of the parameter $\alpha = J_2/J_1$, and vanishes at a critical point α_c, which implies a quantum phase transition between two different VBS state. Since the VBS states of the mixed spin chains actually contain an ensemble of spin singlet state which can be regards as the abundance quantum information resource. It is very desirable to study how the parameter α affects the entanglement of this model or what is the relation between the gapped excitation and the thermal entanglement.

We study both the ground state entanglement and the thermal state entanglement of this system. The state of a quantum system at thermal equilibrium can be described by the density operator $\rho = \frac{1}{Z}\exp(-\beta H)$, where $\beta = \frac{1}{k_B T}$ with k_B the Boltzmann's constant. $Z = \mathrm{Tr}e^{-\beta H}$ is the partition function. The entanglement in the ground state or thermal state is called ground state entanglement or thermal entanglement, respectively. For antiferromagnetic mixed spin chains, the ground state is not degenerate. So the ground state can be directly expressed by the density operator $\rho = \frac{1}{Z}\exp(-\beta H)$ with $\beta \to \infty$. By utilizing the SU(2) invariance of this system, the reduced density matrix $\rho^{(1,1)}$ for two spins $\frac{1}{2}$ or $\rho^{(1,2)}$ for one spin $\frac{1}{2}$ and one spin 1 can be obtained as follows [15]:

$$\rho^{(1,1)} = g^{(1,1)}|0,0\rangle\langle 0,0| + \frac{1-g^{(1,1)}}{3}\sum_{i=-1}^{1}|1,i\rangle\langle 1,i|, \quad (2)$$

and

$$\rho^{(1,2)} = \frac{g^{(1,2)}}{2}\sum_{i=-1/2}^{1/2}|\frac{1}{2},i\rangle\langle\frac{1}{2},i| + \frac{1-g^{(1,2)}}{4}\sum_{i=-3/2}^{3/2}|\frac{3}{2},i\rangle\langle\frac{3}{2},i|, \quad (3)$$

where $|J, J_z\rangle$ denotes the state of total spin J and z component J_z, and $g^{(1,1)}$ and $g^{(1,2)}$ are the function of temperature. For characterizing the ground state pairwise entanglement and the thermal state pairwise entanglement, we adopt the log-negativity as the entanglement measure, which has been proven to be an operational good entanglement measure. The log-negativity $N(\rho_r)$ for the two particle reduced density operator ρ_r is defined as [39]

$$N(\rho_r) = \log_2 \|\rho_r^\Gamma\|, \quad (4)$$

where ρ_r^Γ is the partial transpose of ρ_r and $\|\rho_r^\Gamma\|$ denotes the trace norm of ρ_r^Γ, which is the sum of the singular values of ρ_r^Γ. For the isotropic mixed spin chains with SU(2) symmetry, the log-negativity between any two spins can be proven to be directly related with the two-particle correlation function. Therefore, we can directly calculate the log-negativity by slightly changing the program for the QMC. In Fig.2, we numerically calculate the log-negativity $N^{(1,1)}$ of the reduced density operator of two nearest-neighbor spin $\frac{1}{2}$ in a unit cell of the ground state and the log-negativity $N^{(1,2)}$ of two nearest-neighbor different spin $\frac{1}{2}$ and 1. It is shown that $N^{(1,1)}$ decreases from 1 to zero as the parameter α increases from 0 to 1. At the point of VBS phase transition labelled by $\alpha_c \simeq 0.768$, the entanglement experience a sharply descent. While the entanglement between two nearest-neighbor different spins $\frac{1}{2}$ and 1 characterized by log-negativity $N^{(1,2)}$ is zero for small values of α, and near the critical point it increases with α and experience a sharply ascent at the critical point. Unfortunately, we find that the ground state entanglement only exists between two spins in the same unit cell. In the numerical calculation of the log-negativity of the ground state, we have set $\beta = 200$ and $N = 128$. We conjecture that the descent or ascent of log-negativity near the critical point can be more sharp if the value of β is chosen very very large, though this can consume more and more computation time. From Fig.2, one

can imagine that the quantum mixed spin chain in zero temperature can be utilized as a very good entanglement switch by controlling the parameter α. Recently, Pachos and Plenio have shown that some kinds of atomic lattice can be use to simulation the Hamiltonian of various controllable Heisenberg spin chain [25]. It can motivate us to realize the quantum mixed spin chain in the system of atomic lattice. Then we easily obtain the quantum mixed spin chain with controllable parameter α. The details of suggestion is discussed elsewhere.

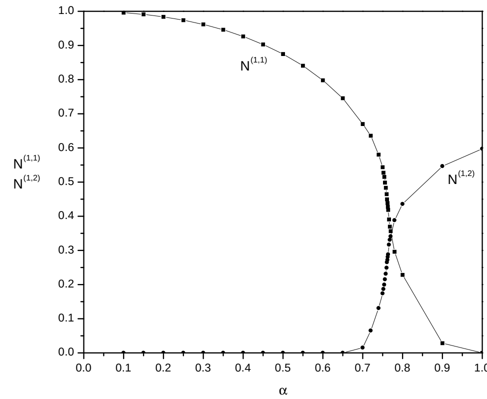

FIG. 2: The log-negativity $N^{(1,1)}$ of the reduced density operator of two nearest-neighbor spin $\frac{1}{2}$ in a unit cell of the ground state and the log-negativity $N^{(1,2)}$ of two nearest-neighbor different spin $\frac{1}{2}$ and 1 are plotted as the function of α. The leng
tem

III. The thermal state entanglement of quantum mixed spin chain

In what follows, we turn to consider the thermal entanglement of the mixed spin chain. In Fig.3, we calculate the log-negativity $N^{(1,1)}$ characterizing the entanglement of two nearest-neighbor as the function of k_BT. It is shown that, if the parameter α is smaller than the critical point α_c, the entanglement decreases with the temperature and vanishes when the temperature goes beyond a threshold value. However, in the cases with $\alpha > \alpha_c$, the entanglement firstly increases with temperature and achieves a local maximal value, then decreases with temperature and eventually vanishes. We can also find that in the cases with low temperature, the entanglement between two nearest-neighbor spin $\frac{1}{2}$ significantly decreases with α. It is natural to conjecture that the thermal state entanglement is closely related with fact whether this system has the gapped excitation.

In Fig.4, we plotted the log-negativity $N^{(1,2)}$ as the function of k_BT for three different values of α near the critical point. Being distinct from the entanglement of two spin $\frac{1}{2}$, if the parameter α is larger than the critical point, the entanglement between two nearest-neighbor different spin $\frac{1}{2}$ and 1 decreases with the temperature and vanishes when the temperature goes beyond another threshold value which is about half of the threshold value concerning the two spin $\frac{1}{2}$. In the case with $\alpha < \alpha_c$, the entanglement of spin 1/2 and spin 1 firstly increases with the temperature, and achieves a local maximal value and then decreases with temperature. From Fig.4, we can also find that the thermal entanglement increases with α, which is consistent with the ground state entanglement.

For more deeply understanding the relation between thermal entanglement and the gapped excitation, the analysis of the entanglement of the excited state of the quantum mixed spin chain is necessary. In what follows, we briefly present a simple numerical method to calculate the log-negativity of the first excited state. In fact, the reduced density matrix of two spins in the first excited state can be obtained by the following procedure.

$$\rho = \frac{1}{Z}e^{-\beta H} \approx \frac{1}{Z}(e^{-\beta E_g}|g\rangle\langle g| + e^{-\beta E_1}|e_1\rangle\langle e_1|) \qquad (5)$$

if the temperature is very very low. Then the reduced density matrix of any two spins can also be expressed as the weight sum of the reduced density matrices of the ground state and the first excited state. By iterating this procedure, we can obtain the log-negativity of two spins in any excited state. The details of this work will be presented elsewhere.

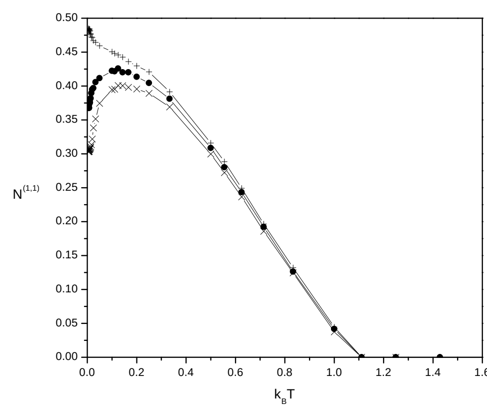

FIG. 3: The log-negativity $N^{(1,1)}$ of the reduced density operator of two nearest-neighbor spin $\frac{1}{2}$ in a unit cell of the thermal state is plotted as the function of k_BT. The length of the lattice sites is chosen as $N = 128$. From top to bottom, $\alpha = 0.758, 0.768, 0.778$, respectively.

V. CONCLUSSION

In this paper, we we investigate the ground state entanglement of the mixed spin chain up to 128 sites by exploring the log-negativity as an entanglement measure. Two distinct behaviors of pairwise entanglement are found. We provide a evidence that the ground state entanglement between two 1/2 spins or between 1/2 spin and 1 spin are closely related to the so-called VBS phase transition. At the point of VBS phase transition, the ground

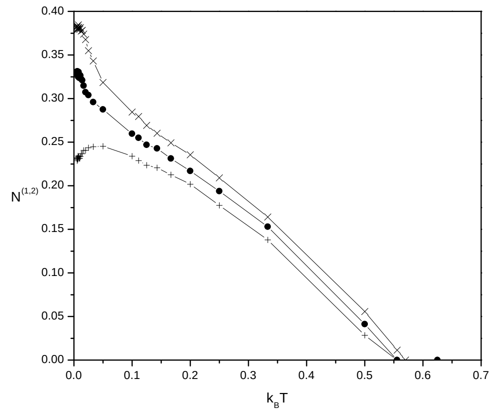

FIG. 4: The log-negativity $N^{(1,2)}$ of the reduced density operator of two nearest-neighbor spin $\frac{1}{2}$ and 1 in a unit cell of the thermal state is plotted as the function of k_BT. The length of the lattice sites is chosen as $N = 128$. From top to bottom, $\alpha = 0.778, 0.768, 0.758$, respectively.

state between two 1/2 spins can be transferred to two different kinds of spins i.e. the spin 1/2 and spin 1 or vice versa. Furthermore, the thermal state pairwise entanglement is also studied and whether the thermal entanglement can be improved by increasing the temperature or not is also addressed, which strongly depends on the parameter $\alpha = J_2/J_1$. It is shown that $N^{(1,1)}$ decreases from 1 to zero as the parameter α increases from 0 to 1. At the point of VBS phase transition labelled by $\alpha_c \simeq 0.768$, the entanglement experience a sharply descent. While the entanglement between two nearest-neighbor different spins $\frac{1}{2}$ and 1 characterized by log-negativity $N^{(1,2)}$ is zero for small values of α, and near the critical point it increases with α and experience a sharply ascent at the critical point. Unfortunately, we find that the ground state entanglement only exists between two spins in the same unit cell. In the numerical calculation of the log-negativity of the ground state, we have set $\beta = 200$ and $N = 128$. if the parameter α is smaller than the critical point α_c, the entanglement decreases with the temperature and vanishes when the temperature goes beyond a threshold value. However, in the cases with $\alpha > \alpha_c$, the entanglement firstly increases with temperature and achieves a local maximal value, then decreases with temperature and eventually vanishes. We can also find that in the cases with low temperature, the entanglement between two nearest-neighbor spin $\frac{1}{2}$ significantly decreases with α. Being distinct from the entanglement of two spin $\frac{1}{2}$, if the parameter α is larger than the critical point, the entanglement between two nearest-neighbor different spin $\frac{1}{2}$ and 1 decreases with the temperature and vanishes when the temperature goes beyond another threshold value which is about half of the threshold value concerning the two spin $\frac{1}{2}$. In the case with $\alpha < \alpha_c$, the entanglement of spin 1/2 and spin 1 firstly increases with the temperature, and achieves a local maximal value and then decreases with temperature. It is natural to conjecture that the thermal state entanglement is closely related with fact whether this system has the gapped excitation.

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